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1987 J. Phys. A: Math. Gen. 20 L77

(http://iopscience.iop.org/0305-4470/20/2/007)

J. Phys. A: Math. Gen. **20** (1987) L77-L83. Printed in the UK

LETTER TO THE EDITOR

Scaling in reaction–diffusion systems

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Received 1 October 1986

Abstract. We study irreversible reaction-diffusion models of the form $pX \overset{k_1}{\leftarrow} mX \overset{k_2}{\rightarrow} qX$, $sX \overset{k_3}{\leftarrow} nX$, $m < n$. Competition between k_1, k_2 gives a continuous transition for $d > d_c = 2(n-m+1)/(n-1)$ which we study for $d < d_c$ using the renormalisation group in conjunction with ε expansion and exact techniques. For $m = 1$ and any n the transition remains continuous. We present ε expansions for the case $n = 3$. By contrast, for $m = 2$ and any n the system shows a fluctuation-induced first-order transition.

Scaling in non-equilibrium irreversible kinetic growth models such as diffusion-limited aggregation (Witten and Sander 1983) and the Eden model (Eden 1961) has led to renewed interest in the properties of simple reaction-diffusion models (Elderfield 1985a, Peliti 1985). As the oft-studied models of Schlögl (1972) have already shown, the absence of simple potential solutions leads to a wealth of rich dynamical structures. We study here the simplest *fully irreversible* reaction-diffusion model which, at the mean-field level of approximation, displays a continuous transition. Adopting a powerful field theoretical approach recently developed (Elderfield 1985b, Grassberger and Scheunert 1980, Peliti 1985), we study our model system using the renormalisation group. Work is done both in the context of ε expansions and *exact* renormalisation group equations. Broadly speaking, the behaviour of these irreversible models falls into two classes. The first is closely related to that of Schlögl (Elderfield and Vvedensky 1985 and references therein), in that ε expansions can be developed and no simple fluctuation dissipation theorem exists. Three critical exponents suffice to determine the full scaling behaviour, despite the suggestion of Ohtsuki and Keyes (1986). For the second class *exact* renormalisation group equations show that no stable fixed point, perturbative or otherwise, exists for $d < d_c$ (the upper critical dimension), indicating the appearance of a fluctuation-driven discontinuous transition.

We consider the irreversible reaction sequence

$$\begin{aligned} &pX \overset{k_1}{\leftarrow} mX \overset{k_2}{\rightarrow} qX \\ &sX \overset{k_3}{\leftarrow} nX \end{aligned} \tag{1}$$

where $m < n$, $p < m < q$, $s < n$. The natural reaction-diffusion master associated with (1) takes the following spatially discrete form:

$$\frac{\partial P}{\partial t}(\{x_i\}, t) = \sum_{ij=1}^{N} D_{ij}((x_i+1)P(x_1, x_2, \ldots, x_i+1, \ldots, x_j-1, \ldots, x_N, t) - P(\{x_i\}, t))$$

0305-4470/87/020077+07$02.50

$$+\sum_{i=1}^{N} k_1\left(\frac{(x_i+m-p)!}{(x_i-p)!}P(x_1,\ldots,x_i+m-p,\ldots,x_N,t)-\frac{x_i!}{(x_i-m)!}P(\{x_i\},t)\right)$$
$$+\sum_{i=1}^{N} k_2\left(\frac{(x_i+m-q)!}{(x_i-q)!}P(x_1,\ldots,x_i+m-q,\ldots,x_N,t)-\frac{x_i!}{(x_i-m)!}P(\{x_i\},t)\right)$$
$$+\sum_{i=1}^{N} k_3\left(\frac{(x_i+n-s)!}{(x_i-s)!}P(x_1,\ldots,x_i+n-s,\ldots,x_N,t)-\frac{x_i!}{(x_i-n)!}P(\{x_i\},t)\right) \quad (2)$$

where x_i is the number of X molecules in the ith cell, the non-local terms represent cell to cell diffusion and the local terms are specified by the reaction sequence. To solve (2) we seek solutions in the form of a Poisson transform (Gardiner and Chaturvedi 1977, Elderfield 1985a),

$$P(\{x_i\},t)=\int_{\mathscr{C}}\prod_{i=1}^{N}\left(\mathrm{d}\alpha_i\exp(-\alpha_i)\frac{\alpha_i^{x_i}}{x_i!}\right)f(\{\alpha_i\},t) \quad (3)$$

where $\mathscr{C}$ is a closed contour in the complex plane and as such $f(\{\alpha_i\},t)$ is best viewed as a Markovian quasiprobability. Direct substitution of (3) into (2) then leads to an *exact* Fokker-Planck description:

$$\frac{\partial f}{\partial t}(\{\alpha_i\},t)=-\sum_{ij}^{N}\frac{\partial}{\partial\alpha_i}(D_{ij}\alpha_j f(\{\alpha_i\},t))-\sum_{i}^{N}\left[k_1\left(\left(1-\frac{\partial}{\partial\alpha_i}\right)^m-\left(1-\frac{\partial}{\partial\alpha_i}\right)^p\right)\right.$$
$$\left.-k_2\left(\left(1-\frac{\partial}{\partial\alpha_i}\right)^q-\left(1-\frac{\partial}{\partial\alpha_i}\right)^m\right)\right]\alpha_i^m f(\{\alpha_i\},t)$$
$$-\sum_{i}^{N}k_3\left(\left(1-\frac{\partial}{\partial\alpha_i}\right)^n-\left(1-\frac{\partial}{\partial\alpha_i}\right)^s\right)\alpha_i^n f(\{\alpha_i\},t) \quad (4)$$

which for our purposes is then best rewritten in a path integral form. Adopting a variant of the Martin-Siggia-Rose (MSR) formalism one obtains a generating functional $Z(\hat{l},l)$ for the Poissonian correlation and response functions in the form (Elderfield 1985b, Elderfield and Vvedensky 1986)

$$Z(\hat{l},l)=\int[\mathrm{d}\hat{\alpha}]\int[\mathrm{d}\alpha]\exp\left(\int\mathrm{d}t(L+l\alpha+\hat{l}\hat{\alpha})\right) \quad (5)$$

where the Lagrangian is given by

$$L=\int\mathrm{d}r^{\alpha}\left[\mathrm{i}\hat{\alpha}(r,t)\left(-D_0\nabla^2+\frac{\partial}{\partial t}\right)\alpha(r,t)\right.$$
$$-k_1((1-\mathrm{i}\hat{\alpha}(r,t))^m-(1-\mathrm{i}\hat{\alpha}(r,t))^p)\alpha^m(r,t)$$
$$+k_2((1-\mathrm{i}\hat{\alpha}(r,t))^q-(1-\mathrm{i}\hat{\alpha}(r,t))^m)\alpha^m(r,t)$$
$$\left.-k_3((1-\mathrm{i}\hat{\alpha}(r,t))^n-(1-\mathrm{i}\hat{\alpha}(r,t))^s)\alpha^n(r,t)\right]. \quad (6)$$

As one might expect Poisson correlation and response functions are given by

$$\langle\alpha(r,t)\rangle=\left.\frac{\partial Z(\hat{l},l)}{\partial l(r,t)}\right|_{\hat{l}=l=0}$$
$$\langle\alpha(r,t)\alpha(r',t')\rangle=\left.\frac{\partial^2 Z(\hat{l},l)}{\partial l(r,t)\,\partial l(r',t')}\right|_{\hat{l}=l=0}. \quad (7)$$

These may then be directly related to the concentration correlation functions via equal-time connection formulas evident from (3):

$$\begin{aligned} &\langle\!\langle x(\boldsymbol{r}, t)\rangle\!\rangle = \langle \alpha(\boldsymbol{r}, t)\rangle \\ &\langle\!\langle x(\boldsymbol{r}, t)x(\boldsymbol{r}', t)\rangle\!\rangle = \langle \alpha(\boldsymbol{r}, t)\alpha(\boldsymbol{r}', t)\rangle + \delta(\boldsymbol{r}-\boldsymbol{r}')\langle \alpha(\boldsymbol{r}, t)\rangle \\ &\qquad\vdots \qquad\qquad\qquad\qquad \vdots \end{aligned} \tag{8}$$

or for multitime correlations by the generalisations derived by Elderfield (1985b)

$$\langle\!\langle x(\boldsymbol{r}, t)x(\boldsymbol{r}', t')\rangle\!\rangle \overset{t>t'}{=} \langle \alpha(\boldsymbol{r}, t)\alpha(\boldsymbol{r}', t)\rangle + \mathrm{i}\langle \alpha(\boldsymbol{r}, t)\hat{\alpha}(\boldsymbol{r}', t')\alpha(\boldsymbol{r}', t')\rangle. \tag{9}$$

On a technical level please note that there are no 'Jacobian' factors in (6) since we have adopted an ordering such that

$$\langle \hat{\alpha}(t)^p \alpha(t)^q\rangle = 0 \tag{10}$$

for all $p > 1$ and any q (Elderfield 1985c). Our representation (5) and (6) is, of course closely related to that of Grassberger and Scheunert (1980) and Peliti (1985). However, for 'factorial' master equations of the form (1) the approach via Poisson transforms seems to offer both the benefits of physical interpretation (Elderfield and Vvedensky 1986) and simplicity. In particular we would note that only in the paper of Elderfield (1985b) can one find information about the multitime correlation functions (9).

Given the Lagrangian L, it is self-evident (if not before) that competition between (k_1, k_2) can lead to a continuous transition from the trivial vacuum $\langle x\rangle = 0$. The deterministic or mean-field approximation gives

$$\partial\alpha/\partial t - D_0\nabla^2\alpha = -(r_0\alpha^m + g_0\alpha^n) \tag{11}$$

where $r_0 \equiv (m-p)k_1 - (q-m)k_2$, $g_0 \equiv (n-s)k_3 > 0$. Extrema of (5) for which $\langle\alpha\rangle = \langle x\rangle < 0$ are unphysical so we need not constrain m to be odd ($m < n$). Solving (11) for non-trivial stationary states one finds directly

$$\langle x\rangle \equiv \langle\alpha\rangle = \begin{cases} (|r_0|/g_0)^{n-m} & r_0 < 0 \\ 0 & \text{otherwise.} \end{cases} \tag{12}$$

Of course, near the phase transition this approximation is of course often poor, since for dimensions $d < d_c$, the upper critical dimension, the corrections to (12) typically diverge as $|r_0| \to 0$. We must therefore estimate d_c and then systematically improve (11) and (12).

To correct (12), we adopt the renormalisation group approach. First we analyse the naive dimensions of the various non-linear couplings in terms of a microscopic time τ and related diffusion length $l = (D_0\tau)^{1/2}$ by observing that

$$[\omega_0] \sim [D_0 k^2] \sim \tau^{-1} \qquad [\hat{\alpha}\alpha] \sim l^{-d} \tag{13}$$

whilst the strongest non-linearities determine (self-consistently) the relative dimension of the fields

$$[\hat{\alpha}(\alpha)^n] \sim [(\hat{\alpha})^2(\alpha)^m] \tag{14}$$

for $n > m$ and $r_0 \to 0$. Using this information we can follow Brézin *et al* (1973) and now focus on the reduced Lagrangian L^*

$$L^* = \int \mathrm{d}\boldsymbol{r}^d \left\{ \mathrm{i}\hat{\alpha}\left[\left(\frac{\partial}{\partial t} - D_0\nabla^2\right)\alpha + r_0\alpha^m + g_0\alpha^n\right] + v_0\hat{\alpha}^2\alpha^m \right\} \tag{15}$$

where the dominant non-linear couplings g_0, v_0 have dimension

$$[g_0]=[v_0]\sim \tau^{-1}l^{d(n-1)/(n-m+1)}. \tag{16}$$

As usual the upper critical dimension d_c follows from consideration of the associated dimensionless coupling:

$$z\equiv (g_0/D)(\zeta)^{2-d(n-1)/(n-m+1)}. \tag{17}$$

Here the length ζ, divergent as the transition is approached, is a characteristic macroscopic length. For $r_0<0$ or $m=1$, ζ can be taken to be the correlation length but for other cases one must be more careful. Corrections to (12) are controlled by (17) so it is self-evident that, for $d<d_c$,

$$d_c=\frac{2(n-m+1)}{n-1} \tag{18}$$

mean-field approximations must be abandoned. Higher-order couplings dropped from (15) by the same token give only finite corrections. As a final cosmetic feature we observe that by a simple finite rescaling we may set $|g_0|=|v_0|$, so we replace L^* by L:

$$L_{\pm}=\int \mathrm{d}\boldsymbol{r}^d\left[\mathrm{i}\hat{\alpha}\left(\frac{\partial\alpha}{\partial t}-D_0\nabla^2\alpha+r_0\alpha^m\right)+g_0(\mathrm{i}\hat{\alpha}\alpha^n\pm\hat{\alpha}^2\alpha^m)\right]. \tag{19}$$

Stripped of irrelevant details it is this Lagrangian, rather than L defined by (6), that controls the physics of the reaction scheme (1).

To construct the desired renormalisation group equation we use a variant of the approach of de Dominicis and Peliti (1978). First we renormalise the theory by defining new fields α_R, $\hat{\alpha}_R$ and couplings D, r, g, v:

$$\begin{aligned}
&\hat{\alpha}_R=(\hat{Z}/Z)\hat{\alpha}\\
&\alpha=Z\alpha\\
&D_0=D(Z_D/\hat{Z}) \qquad\qquad r_0=r(Z_r/\hat{Z})Z^{1-m}\\
&g_0=g\tau^{-1}(D\tau)^{\frac{1}{2}[d(n-1)/(n-m+1)]}Z_g\hat{Z}^{-1}Z^{1-n}\\
&v_0=v\tau^{-1}(D\tau)^{\frac{1}{2}[d(n-1)/(n-m+1)]}Z_v\hat{Z}^{-2}Z^{2-m}
\end{aligned} \tag{20}$$

which after fixing the Z by minimal subtraction on the dimensionally regularised theory renders the theory finite (Amit 1978). Introducing the vertex generator

$$\Gamma(\hat{M},M)\equiv \ln Z(\hat{l},l)-\hat{M}\hat{l}-Ml\equiv\sum\frac{(\hat{M})^k}{k!}\frac{M^p}{p!}\Gamma^{(\wedge)^k,(-)^p} \tag{21}$$

one has by construction the relation

$$\Gamma(\hat{M}_R,M_R,D,r,g,v,\tau)=\Gamma(\hat{M},M,D_0,r_0,g_0,v_0) \tag{22}$$

which amounts to a renormalisation group equation once the Z have been determined. To fix all the Z with the exception of the field renormalisation Z, it is sufficient to renormalise the vertex functions

$$\frac{\partial\Gamma^{\wedge-}}{\partial q^2},\frac{\partial\Gamma^{\wedge-}}{\partial(\mathrm{i}\omega)},\left(\frac{\partial\Gamma^{\wedge(-)^m}}{\partial r_0}\right)_{r_0=0},\Gamma^{\wedge(-)^n},\Gamma^{(\wedge)^2(-)^m}. \tag{23}$$

In order to fix Z we observe that the initial rescaling symmetry, by which we chose $v_0 = g_0$, implies from (20)

$$g/v = (Z_v/Z_g)(\hat{Z})^{-1} Z^{n-m+1}. \tag{24}$$

Naturally in the renormalised theory we may also choose $g = v$, providing then that Z is chosen consistently from (24). Other choices are equivalent up to irrelevant reparametrisations, whilst $g = v$ has great merit in that the non-linear coupling controlling the physics is unique. Given (22) and $g = v$, we may obtain the renormalisation group equation by simple differentiation. One finds

$$\left[\tau\frac{\partial}{\partial\tau} + \beta(g)\frac{\partial}{\partial g} + \left(\frac{1}{\nu z(g)} + \frac{2}{z(g)}\frac{d}{d_c}\left(\frac{m-1}{n-1}\right) - 1\right) r\frac{\partial}{\partial r} + \left(\frac{2}{z(g)} - 1\right) D\frac{\partial}{\partial D} + \tfrac{1}{2}\hat{\eta}(g)\hat{M}\frac{\partial}{\partial \hat{M}} + \tfrac{1}{2}\eta M\frac{\partial}{\partial M}\right]\Gamma = 0 \tag{25}$$

where

$$\beta(g,\varepsilon) = \left(\frac{\partial g}{\partial \ln \tau}\right)_{g_0, r_0, D_0} = \left(1 - \frac{1}{2}\frac{d(n-1)}{(n-m+1)}\right)\frac{\partial g}{\partial \ln g_0}$$

$$\left[\frac{1}{\nu(g)z(g)} + \frac{2}{z(g)}\left(\frac{d}{d_c}\right)\left(\frac{m-1}{n-1}\right) - 1\right] = -\beta(g)\frac{\partial}{\partial g}\ln(Z_r/\hat{Z}Z^{m-1})$$

$$\left(\frac{2}{Z(g)} - 1\right) = -\beta(g)\frac{\partial}{\partial g}\ln(Z_D/\hat{Z}) \tag{26}$$

$$\tfrac{1}{2}\eta(g) = \beta(g)\frac{\partial}{\partial g}\ln(Z)$$

$$\tfrac{1}{2}\hat{\eta}(g) = \beta(g)\frac{\partial}{\partial g}\ln(\tilde{Z}/Z)$$

and $\varepsilon = d_c - d$. The exponent functions $\beta(g)$, $\nu(g)$, $z(g)$, $\eta(g)$, $\hat{\eta}(g)$ are of course regular functions of g, ε only.

The renormalisation group equation (25) describes the full scaling behaviour of the theory at large distances and long times. Legendre transformation, functional differentiation and the connection formulae (8) and (9) show (Elderfield and Vvedensky 1985) that, for example, the concentration $\langle x\rangle$ and two-point correlation function $\langle xx\rangle$ satisfy

$$\left[\tau\frac{\partial}{\partial\tau} + \beta(g)\frac{\partial}{\partial g} + \left(\frac{1}{\nu(g)z(g)} + \frac{2}{z(g)}\left(\frac{d}{d_c}\right)\left(\frac{m-1}{n-1}\right) - 1\right) r\frac{\partial}{\partial r} + \left(\frac{2}{z} - 1\right) D\frac{\partial}{\partial D}\right]\begin{pmatrix}\langle x\rangle \\ \langle xx\rangle\end{pmatrix} = \eta(g)\begin{pmatrix}\tfrac{1}{2}\langle x\rangle \\ \langle xx\rangle\end{pmatrix}. \tag{27}$$

(28)

Solution of these equations is standard (Amit 1978). Assuming the existence of an infrared stable fixed point $g^*(\beta(g^*) = 0,\ \beta'(g^*) < 0)$ one finds

$$\langle x\rangle \sim |r|^{\nu[d/(n-m+1)+\frac{1}{2}z\eta]} \tag{29}$$

$$\langle xx\rangle \sim \frac{|r|^{-\nu z(1-R)}}{\langle x\rangle^{n-m-1}} f(q^2/|r|^{2\nu})(\omega/|r|^{\nu z}) \tag{30}$$

where the critical exponents $\nu = \nu(g^*)$, $z = z(g^*)$, $\eta = \eta(g^*)$ are identified. Strictly for the reaction scheme (1), $\hat{\eta}$ is redundant for $\hat{I} \neq 0$ corresponds to addition of a reaction

$$0 \to X. \tag{31}$$

The scaling behaviour of the irreversible system (1) is thus completely described by three critical exponents ν which controls the correlation length, z the dynamical exponent and the anomalous field dimension η.

We have implemented the full renormalisation group programme outlined above for two classes of system.

(*a*) $m = 1$, $n = k$, $d_c = 2k/(k-1)$. Quite generally for these systems one is forced to work within the framework of an ε expansion. We note that for $k = 2$, $d_c = 4$ and the system belongs to the same universality class as Schlögl's first model (Elderfield and Vvedensky 1985 and references therein):

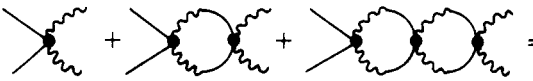
$$\begin{aligned} X &\rightleftharpoons 2X \\ X &\rightleftharpoons 0 \end{aligned} \tag{32}$$

a model which is plainly reversible. In consequence there is an additional symmetry $\hat{\alpha}(t) \rightleftharpoons \alpha(-t)$ which implies $\hat{\Lambda}(g) = \Lambda(g)$. For higher values of k new universality classes appear. In particular, for $k = 3$, $d_c = 3$ and we find three independent critical exponents:

$$\begin{aligned} \nu &= \tfrac{1}{2} - 0.026\varepsilon + O(\varepsilon^2) \\ Z &= 2 + 0.016\varepsilon + O(\varepsilon^2) \\ \Lambda &= 0.010\varepsilon + O(\varepsilon^2) \end{aligned} \tag{33}$$

to leading order in $\varepsilon = 3 - d$. Note that $L_+ \equiv L_-$ in (19) for this case.

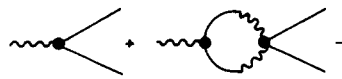
(*b*) $m = 2$, $n = k$, $d_c = 2$. In a real sense these systems are trivial because the renormalisation programme leads to *exact* exponent functions. Diagrammatically one finds that the two-point vertex functions do not renormalise, whilst the higher vertex functions (23) are proportional and may be evaluated directly. Explicitly one has for $L_\pm$ in (19)

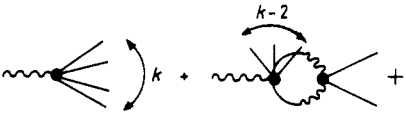
$\Gamma^{\wedge\wedge--}_{\pm} =$  $= \pm \dfrac{g_0}{1 \pm g_0 I}$ (34)

where

$$\frac{I}{\varepsilon} = \int \left(\frac{dq}{2\pi}\right)^d \frac{1}{D(q^2 + (p+q)^2)}\bigg|_{Dp^2\tau=1}$$

and furthermore

$\dfrac{\partial \Gamma^{\wedge--}}{\partial r_0} =$  $= \pm \dfrac{1}{g_0} \Gamma^{\wedge\wedge--}$

$\Gamma^{\wedge(-)^k} =$  $= \pm \Gamma^{\wedge\wedge--}.$ (35)

Consequently there is an infrared stable fixed point only for L_+ for we find

$$\beta^{\pm}(g) = \tfrac{1}{2}\varepsilon g \mp I g^2 \qquad I > 0. \tag{36}$$

Moreover there is but one non-trivial exponent

$$\nu = \frac{1}{d}\frac{(k-1)}{(k-2)}. \tag{37}$$

The sign of v_0, which determines whether L_+ or L_- is appropriate, is therefore of crucial importance. From (b) we observe

$$v_0 = 2k_1 - q(q-1)k_2 \tag{38}$$

so that in the vicinity of the transition $v_0 < 0$ for all $q \geqslant 3$ and thus the unstable Lagrangian L_- is found in all cases. Whence the continuous transition located by mean-field theory in $d < 2$ dimensions becomes first order directly for $d < 2$. For completeness it is perhaps interesting to observe that L_+ is relevant in the exceptional case $k_2 = 0$, $m = n = 2$ corresponding to diffusive annilation (Peliti 1986)

$$2X \to X \to 0. \tag{39}$$

We would like to thank the SERC for support.

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